Bayesian Anomaly Detection for Ia supernovae using JAX-bandflux

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Outline

JAX and JAX-bandflux

Bayesian anomaly detection

Apply on Ia supernovae

JAX and JAX-bandflux

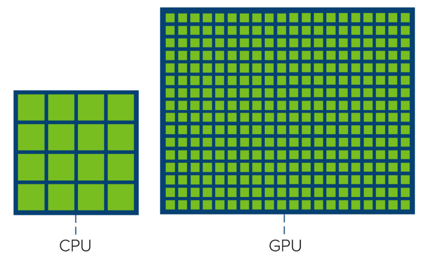
What is JAX

- JAX is a high-performance numerical computing library
- Combines NumPy-like functionality with:
    - Automatic differentiation (like TensorFlow/PyTorch)
    - Just-in-time (JIT) compilation
    - GPU/TPU acceleration
- Fundamentally, allows us to run highly parallelized operations on powerful GPUs

Why do we care about doing things on GPUs

- Massive parallelization capabilities
  - CPUs: Few cores (4-64), high clock speeds
  - GPUs: Thousands of cores, designed for parallel tasks
  - Significant performance improvements for numerical computations

- Useful for astronomical applications
  - Processing large datasets (e.g., supernova surveys)
  - Running complex simulations (e.g., SBI)
  - Performing parameter inference with many samples



Limitations in JAX

- Vectors length must be defined at compilation

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- Limited control flow (no while loops, etc)

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- Vectors length must be defined at compilation
- Limited control flow (no while loops, etc)
- Debugging and optimising is hard

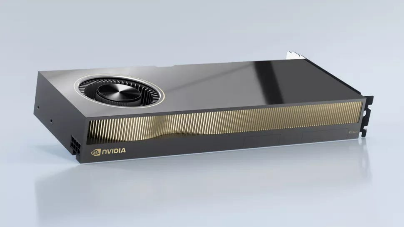
JAX numpy vs numpy

```
import numpy as np
x = np.arange(10)
y = np.zeros_like(x)
for i in range(len(x)):
    y[i] = x[i] * 2
```

```
import jax.numpy as jnp
from jax import vmap
x = jnp.arange(10)
def double(v):
    return v * 2
y = vmap(double)(x)
```

What is JAX bandflux?

sncosmo
A Python Library for Supernova Cosmology



What does JAX-bandflux do?

$$F(p,\lambda) = x_0\big[M_0(p,\lambda) + x_1 M_1(p,\lambda) + \ldots\big] \times \exp\big[c\, CL(\lambda)\big] \tag{1}$$

IN:

- x_0, x_1, t_0, c
- $M_0(p,\lambda), M_1(p,\lambda)$
- p (phase/redshift)
- $CL(\lambda)$

OUT:

- Flux: $F(p,\lambda)$

Bandflux Computation

- Bandflux: Integrated flux through a specific filter

$$\text{bandflux} = \int_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} F(\lambda) \cdot T(\lambda) \cdot \frac{\lambda}{hc} \, d\lambda \tag{2}$$

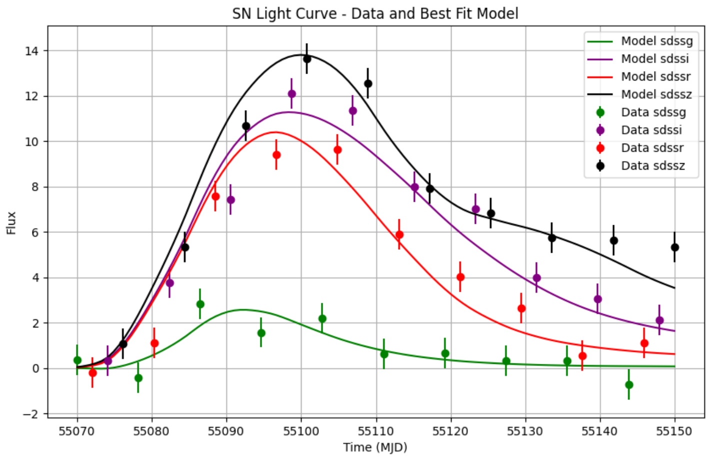
- Components:
  - $F(\lambda)$: Spectral flux density
  - $T(\lambda)$: Filter transmission function
  - $\lambda/(hc)$: Conversion from energy to photon counts
- Implementation in JAX-bandflux:
  - Vectorized array operations
  - JIT-compiled for efficiency
  - Trapezoidal integration along wavelength dimension
  - Parallelized across multiple data instances via `vmap`

Can now construct GPU compatible likelihood

$$\mathcal{L}(\mathbf{F} \mid \theta) = \prod_i \frac{1}{\sqrt{2\pi}\,\sigma_i} \exp\left[-\frac{(F_i - \mu_i(\theta))^2}{2\,\sigma_i^2} \right]$$

- Observed fluxes F_i: measured data; model fluxes $\mu_i(\theta)$: predicted flux given parameters
- With this likelihood we can now perform parameter estimation
- Likelihood is differentiable and can be compiled as part of broader GPU workflows

Can now fit light curves on GPU

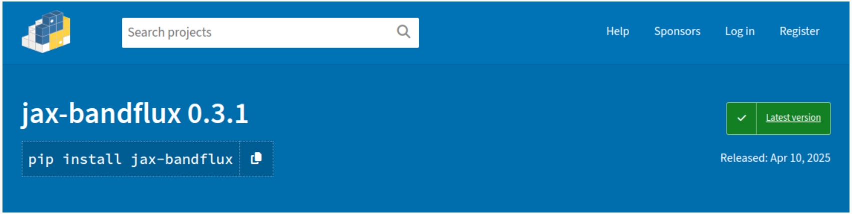


Bandflux Computation Example

- For a detailed walkthrough of bandflux computation:
  - Interactive Jupyter notebook with step-by-step implementation
  - Demonstrates JAX-bandflux API usage
  - Shows performance benefits of GPU acceleration
  - Includes visualization of results
- Access the example notebook:

Supernovae Analysis Example Notebook

PIP installable



JAX-bandflux: differentiable supernovae SALT modelling for cosmological analysis on GPUs

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Bayesian anomaly detection

Over simplified example of anomaly detection method (thresholding)

Simple statistical approach:

- Calculate mean (μ) and standard deviation (σ) of the data
- Define threshold $T = \mu + k\sigma$ where k is a sensitivity parameter
- Flag data point x_i as anomalous if:

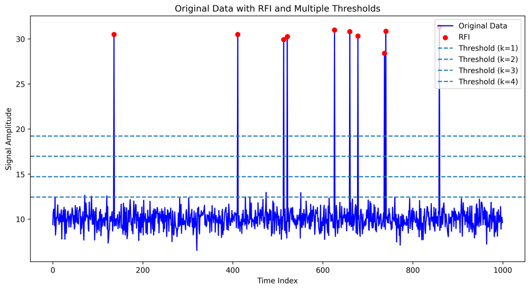
$$\text{anomaly}_i = \begin{cases} 1 & \text{if } x_i > T \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

Limitations:

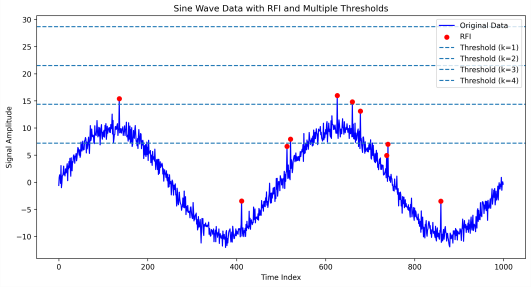
- Choice of k is arbitrary
- Assumes Gaussian statistics
- No consideration of temporal correlations
- Cannot distinguish between RFI and real signals

Thresholding results

Constant signal with RFI:



Sine wave with RFI:



Defining an anomaly sensitive likelihood

a) Generate peicewise likelihood:

$$P(\mathcal{D}_i|\theta) = \begin{cases} \mathcal{L}_i(\theta) & : \text{expected} \\ \Delta^{-1}[0 < \mathcal{D}_i < \Delta] & : \text{anomalous}, \end{cases} \tag{4}$$

b) Ascribe Bernoulli prior:

$$P(\varepsilon_i) = p_i^{(1-\varepsilon_i)}(1-p_i)^{\varepsilon_i}. \tag{5}$$

c) Marginalise over epsilon:

$$P(\mathcal{D}|\theta) = \sum_{\varepsilon \in \{0,1\}^N} P(\mathcal{D}, \varepsilon|\theta) \tag{6}$$

d) Approximate correct mask is most likely

$$P(\mathcal{D}|\theta, \varepsilon_{\max}) \gg \max_j P(\mathcal{D}|\theta, \varepsilon^{(j)}), \tag{7}$$

e) Loglikelihood:

$$\log P(\mathcal{D}|\theta) = \sum_i [\log \mathcal{L}_i + \log(1-p_i)]\varepsilon_i^{\max} + [\log p_i - \log \Delta](1-\varepsilon_i^{\max}) \tag{8}$$

Computing the Posterior

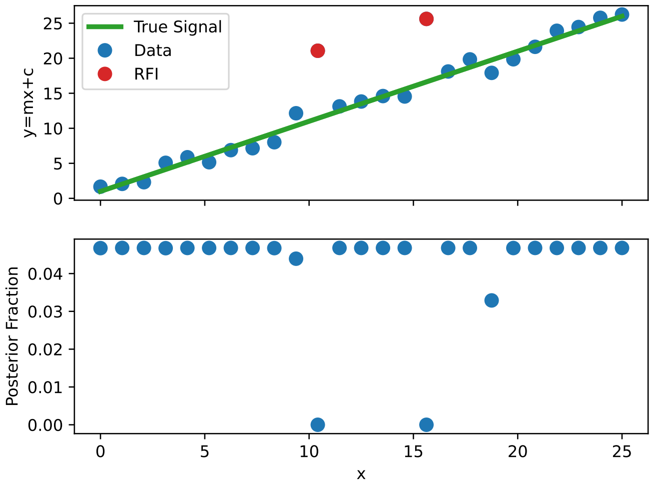
e) Loglikelihood:

$$\log P(\mathcal{D}|\theta) = \sum_i [\log \mathcal{L}_i + \log(1 - p_i)]\varepsilon_i^{\mathrm{max}} + [\log p_i - \log \Delta](1 - \varepsilon_i^{\mathrm{max}}) \tag{6}$$

f) Maximise ε^{max} by comparing the terms:

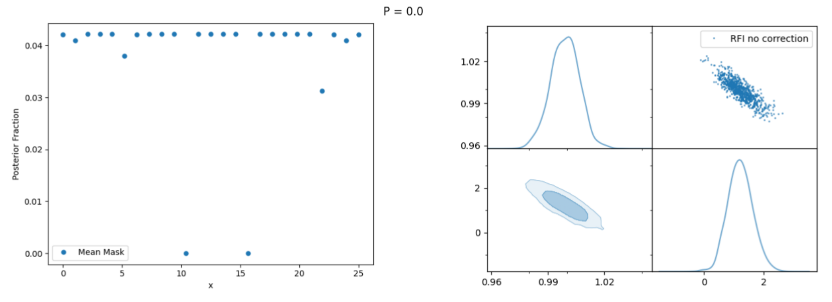
$$\log P(\mathcal{D}|\theta) = \begin{cases} \log \mathcal{L}_i + \log(1 - p_i), & \text{if } [\log \mathcal{L}_i + \log(1 - p_i) > \log p_i - \log \Delta] \\ \log p_i - \log \Delta, & \text{otherwise} \end{cases} \tag{7}$$

Fit on a simple toy model

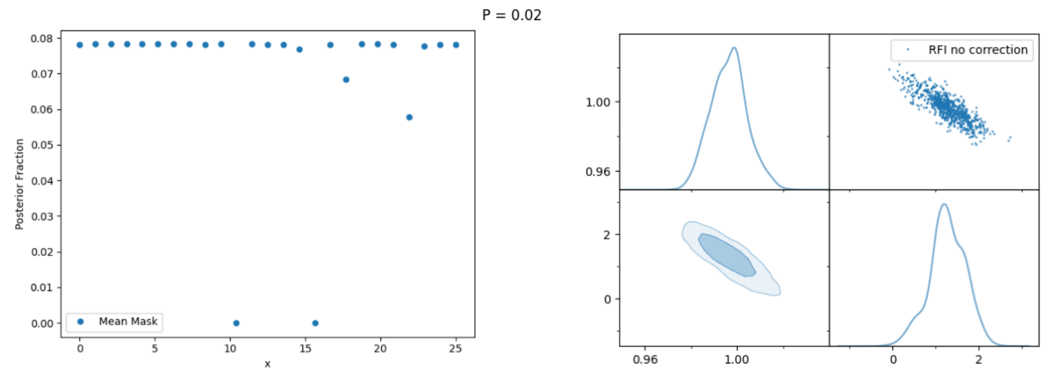


Likelihood thresholding condition p

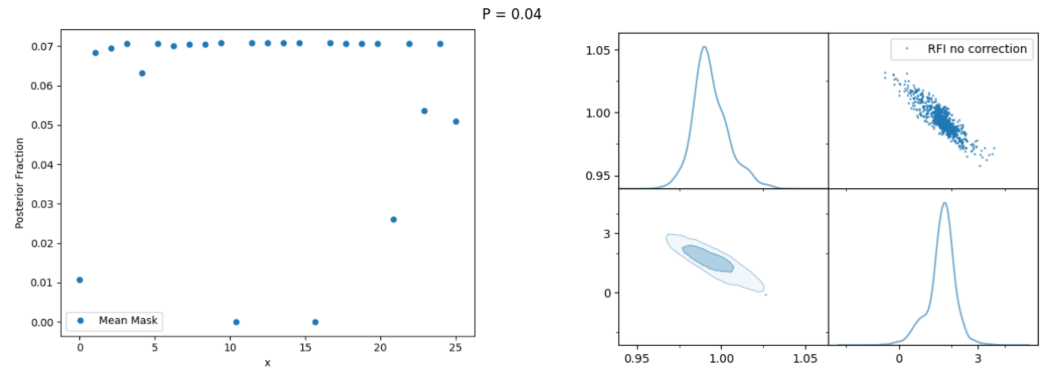
$$\log P(\mathcal{D}|\theta) = \sum_i [\log \mathcal{L}_i + \log(1-p_i)]\varepsilon^{\max} + [\log p_i - \log \Delta](1-\varepsilon_i^{\max}) \tag{9}$$



Varying p


P = 0.02
Posterior Fraction
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
Mean Mask
0
5
10
15
20
25
x
RFI no correction
1.00
0.96
2
0
0.96
1.00
0
2

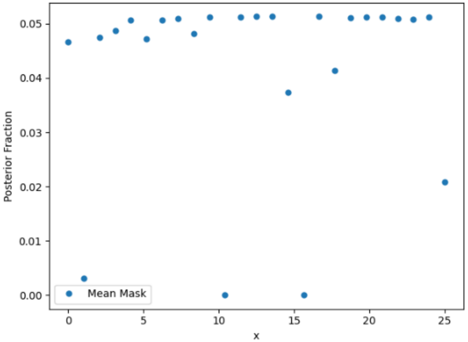
Varying p

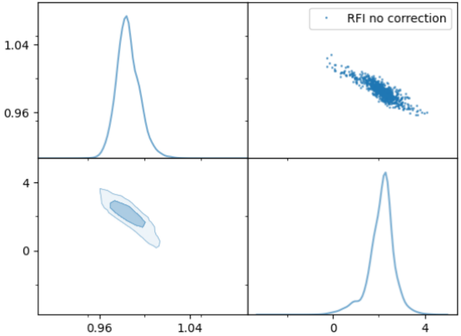


P = 0.04
Posterior Fraction
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
Mean Mask
0
5
10
15
20
25
x
RFI no correction
1.05
1.00
0.95
3
0
0.95
1.00
1.05
0
3

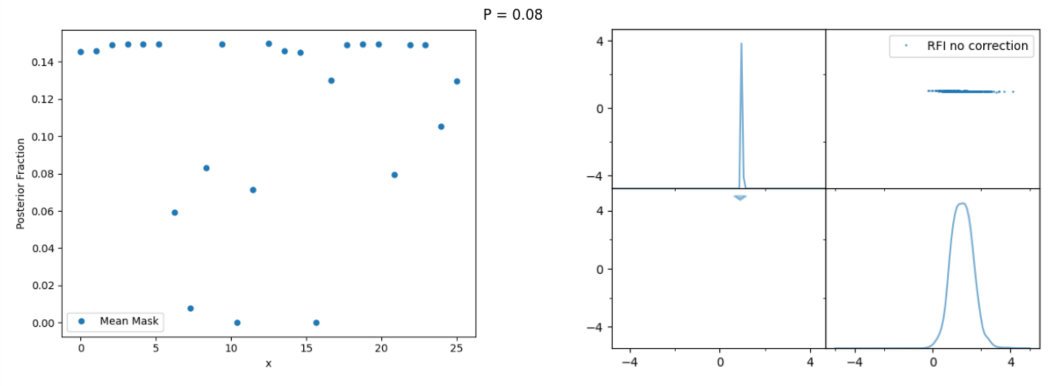
Varying p

P = 0.06



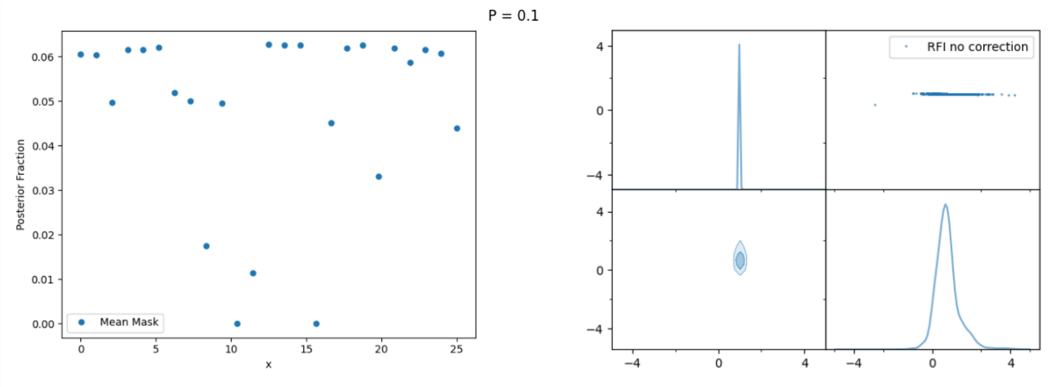


Varying p



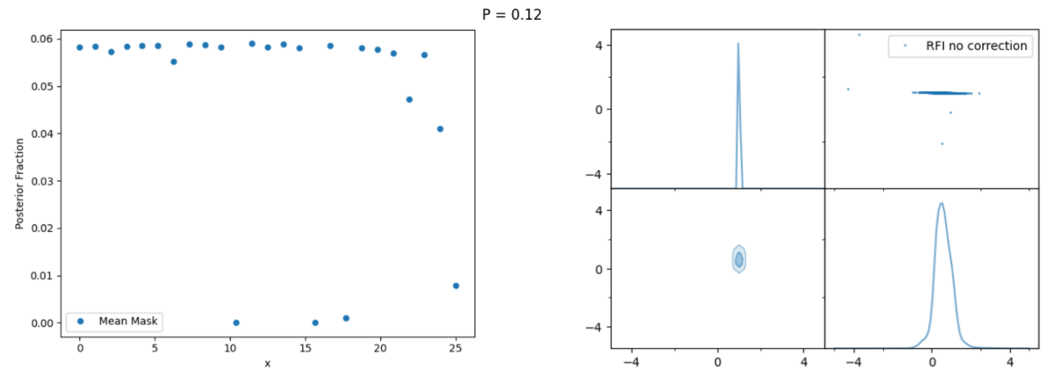
P = 0.08
Posterior Fraction
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
Mean Mask
0
5
10
15
20
25
x
RFI no correction
4
0
−4
4
0
−4
−4
0
4
−4
0
4

Varying p



P = 0.1
Posterior Fraction
0.06
0.05
0.04
0.03
0.02
0.01
0.00
Mean Mask
0
5
10
15
20
25
x
RFI no correction
4
0
−4
4
0
−4
−4
0
4
−4
0
4

Varying p


P = 0.12
Posterior Fraction
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0.01
0.00
Mean Mask
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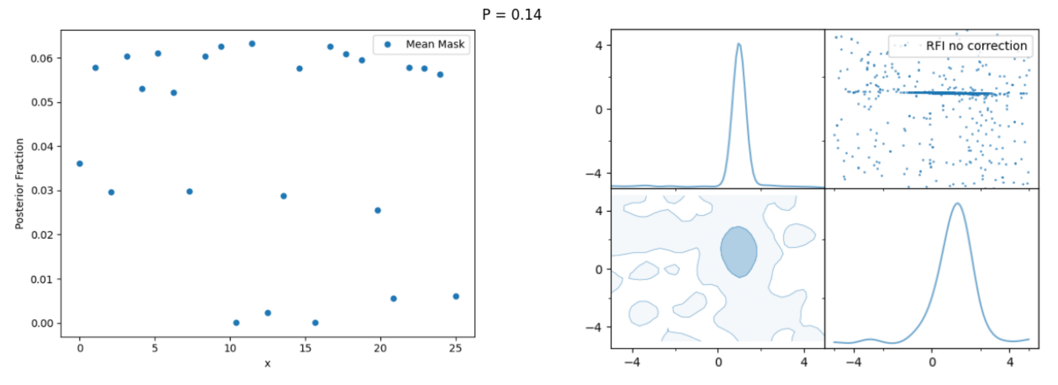
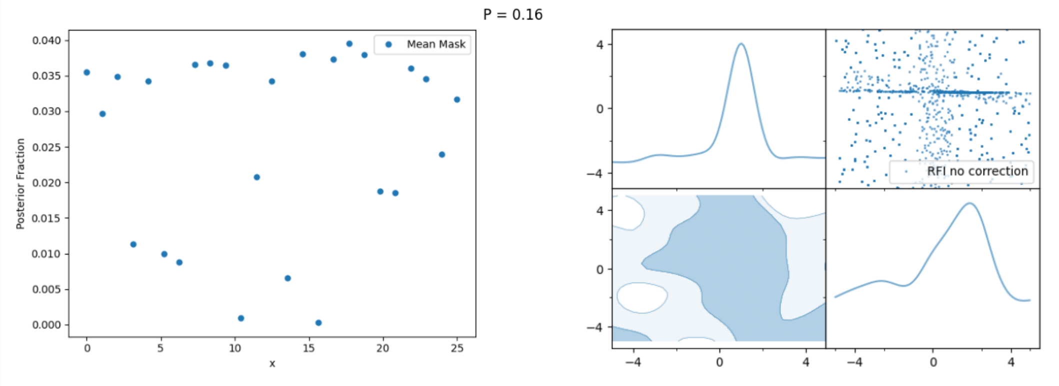
15
20
25
x
RFI no correction
4
0
−4

Varying p


P = 0.14
Mean Mask
Posterior Fraction
0.06
0.05
0.04
0.03
0.02
0.01
0.00
0
5
10
15
20
25
x
RFI no correction
4
0
−4
4
0
−4
−4
0
4
−4
0
4

Varying p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Mean Mask
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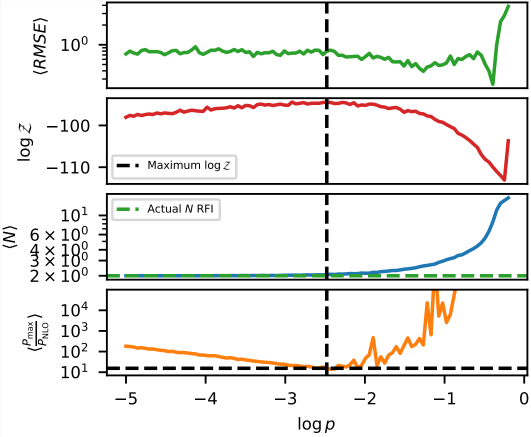
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
0
5
10
15
20
25
RFI no correction
4
0
−4

Selection strategy for p.

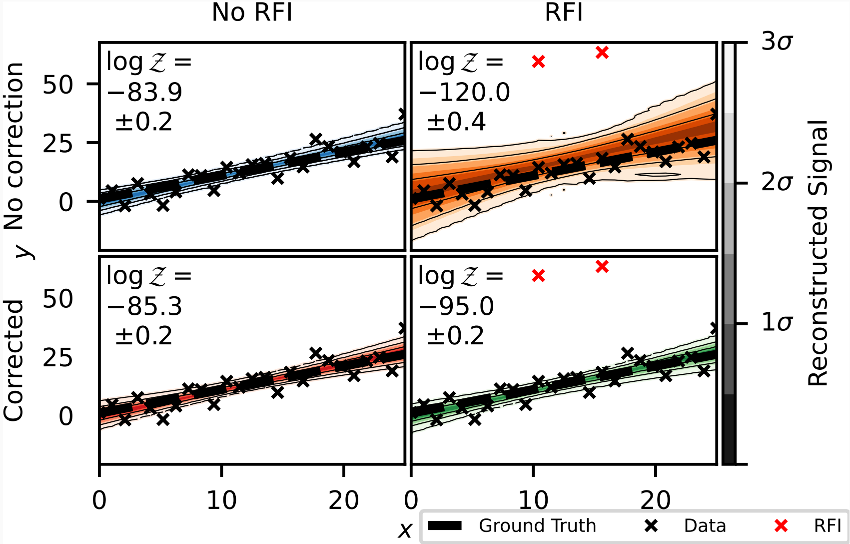
- 'Select p such that the Bayesian evidence is maximised'



Fully automated anomaly detection

- Putting a prior on p, we can fit it dynamically as a free parameter.
- This fully automates the anomaly detection process.
- Must exclude $p = 0$.

Application to toy model



Implement with 2 lines of code

```python
def likelihood(theta):
    sig = theta[0]
    logL = -(f_noise - window)**2/sig**2/2 - np.log(2*np.pi*sig**2)/2
    return logL, []
```

```python
def likelihood(theta):
    sig = theta[0]
    logL = -(f_noise - window)**2/sig**2/2 - np.log(2*np.pi*sig**2)/2 + np.log(1-p)
    emax = logL > logp - np.log(delta)
    logPmax = np.where(emax, logL, logp - np.log(delta)).sum()
    return logPmax, []
```

Tutorial @ github.com/samleeney

Read the paper!

PHYSICAL REVIEW D **108**, 062006 (2023)

Bayesian approach to radio frequency interference mitigation

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Interfering signals such as radio frequency interference from ubiquitous satellite constellations are becoming an endemic problem in fields involving physical observations of the electromagnetic spectrum. To address this we propose a novel data cleaning methodology. Contamination is simultaneously flagged and managed at the likelihood level. It is modeled in a Bayesian fashion through a piecewise likelihood that is constrained by a Bernoulli prior distribution. The techniques described in this paper can be implemented with just a few lines of code.

DOI: 10.1103/PhysRevD.108.062006

arxiv: 2211.15448

Apply on Ia supernovae

Standard vs. Anomaly Detection Likelihoods

Standard Likelihood:

$$\log \mathcal{L}_{\text{std}} = -\frac{1}{2}\sum_i \left(\frac{f_i - m_i}{\sigma_i}\right)^2 - \frac{1}{2}\sum_i \log(2\pi\sigma_i^2) \qquad (10)$$

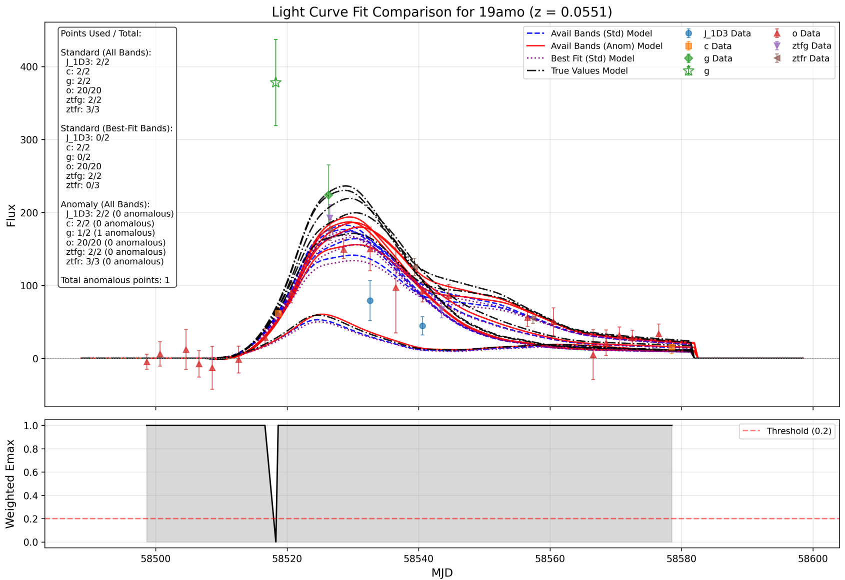
- f_i: Observed flux
- m_i: Model flux (SALT3)
- σ_i: Flux uncertainty

Anomaly Detection Likelihood:

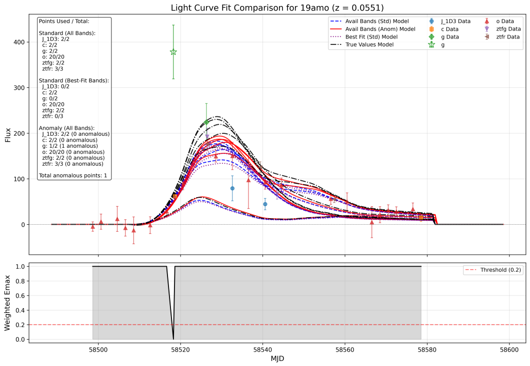
$$\log \mathcal{L}_{\text{anom}} = \sum_i \begin{cases} \log \mathcal{L}_i + \log(1-p), & \text{if } e_i^{\max} \\ \log p - \log \Delta, & \text{otherwi} \end{cases} \qquad (11)$$

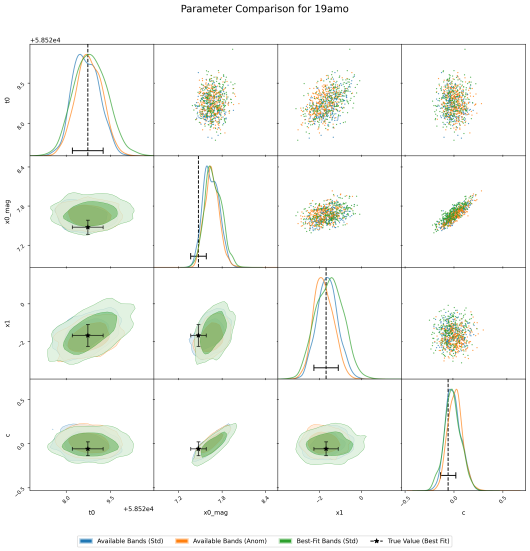
- $\log \mathcal{L}_i$: Point-wise standard likelihood
- p: Anomaly probability (fitted parameter)
- $e_i^{\max}$: Boolean indicating normal data
- Δ: Maximum flux range

Applying to Ia supernovae

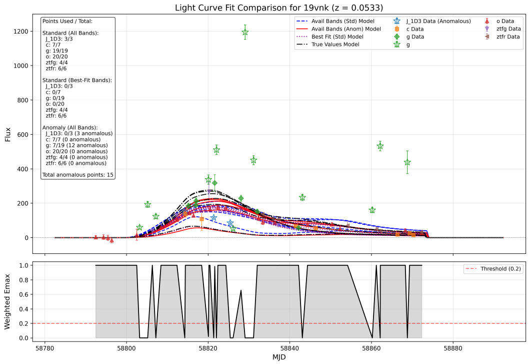


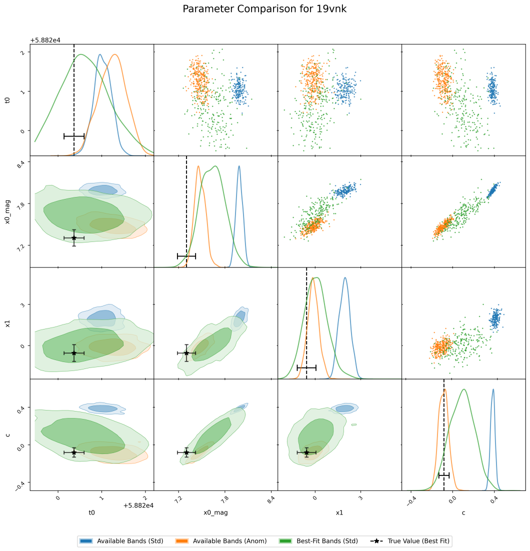
SN 19amo: Classic 'anomaly detection' example



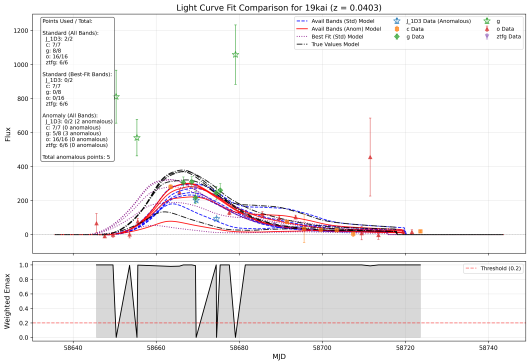


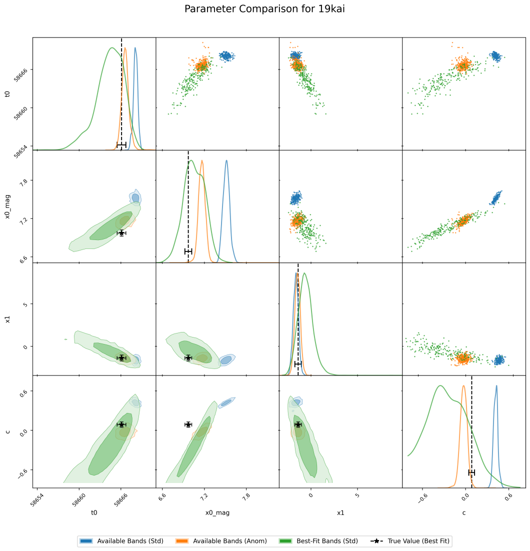
SN 19vnk: Automatic filter removal



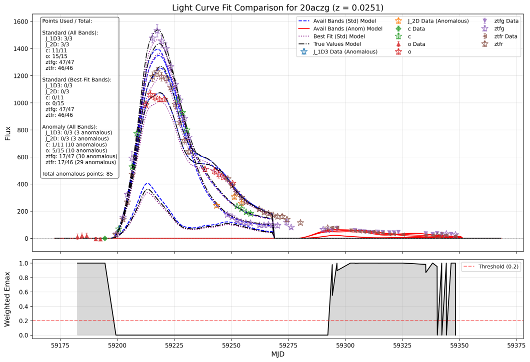


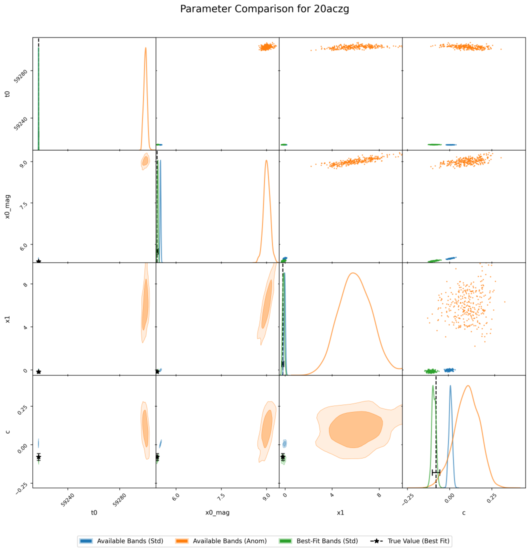
SN 19kai: Flagging while preserving some data





SN 20aczg: Light Curve and Corner Plot Comparison





Key points

1. Standard flagging.

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2. Automated filter selection.

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1. Standard flagging.
2. Automated filter selection.
3. Data preservation from previously discarded filters.
4. Potentially can flag non Ia automatically?

Next steps

- Assess Hubble diagrams
    - Quantify impact on cosmological parameter estimation
    - Compare with traditional outlier rejection methods
    - Evaluate systematic error reduction
- Try on other datasets?
    - Apply to different supernova surveys (ZTF, LSST)
    - Test with different photometric systems
    - Evaluate performance across redshift ranges